

REB, The Course

Class 3 Practice Assignment Solution

A reaction was studied at the temperatures, T , listed in the Table below, and at each temperature the value of the first-order rate coefficient, k , was determined. On the basis of the information provided in the table, does the rate coefficient display Arrhenius temperature dependence? If it does, what are the values of the pre-exponential factor and the activation energy? The data are also available in the file, `practice_3_data.csv`.

$T (^{\circ}F)$	$k (s^{-1})$
76.7	1.12E-05
92.9	3.63E-05
114.5	1.15E-04
132.5	3.26E-04
148.7	8.92E-04

Table 1. Rate coefficient data.

The Arrhenius expression is given in equation (1); taking the log of both sides of the equation leads to equation (2). Equation (2) has the form of a straight line, equation (3) if y and x are defined as given in equations (4) and (5) and if the slope and intercept are as defined in equations (6) and (7).

$$k = k_0 \exp \left(\frac{-E}{RT} \right) \quad (1)$$

$$\ln k = \left(\frac{-E}{R} \right) \left(\frac{1}{T} \right) + \ln k_0 \quad (2)$$

$$y = mx + b \quad (3)$$

$$y = \ln k \quad (4)$$

$$x = \frac{1}{T} \quad (5)$$

$$m = \frac{-E}{R} \quad (6)$$

$$b = \ln k_0 \quad (7)$$

After converting the temperatures to °R, the data in Table 1 were used to calculate corresponding $\underline{x}$ and $\underline{y}$ data. The REB Utility function, Arrhenius_parameters, was used to fit equation (3) to the resulting data. Equation (6) was then used to calculate the estimated activation energy and the upper and lower limits of it's 95% confidence interval from the corresponding values for the slope, m . The pre-exponential factor and its confidence interval were similarly calculated using equation (7) and the estimated intercept, b .

Results and Discussion

The best estimate for the activation energy is $E = 38,590 \text{ BTU lbmol}^{-1}$, 95%CI [35,430, 41750]. That for the pre-exponential factor is $6.07 \times 10^{10} \text{ s}^{-1}$, 95% CI [3.75×10^9 , 9.85×10^{11}]. The coefficient of determination is 0.998, and an Arrhenius plot is shown in Figure 1.

The rate coefficients in Table 1 do display Arrhenius temperature dependence. The coefficient of determination is nearly equal to 1, and the scatter of the data about the line in Figure 1 is small in magnitude and random. The limits of the 95% confidence interval for the activation energy are close to the estimated value. These are all characteristics of an accurate model. The limits of the confidence interval for the pre-exponential factor are much larger, but this is often the case for pre-exponential factors. Overall, the Arrhenius expression provides an acceptably accurate representation of the experimental rate coefficient data.

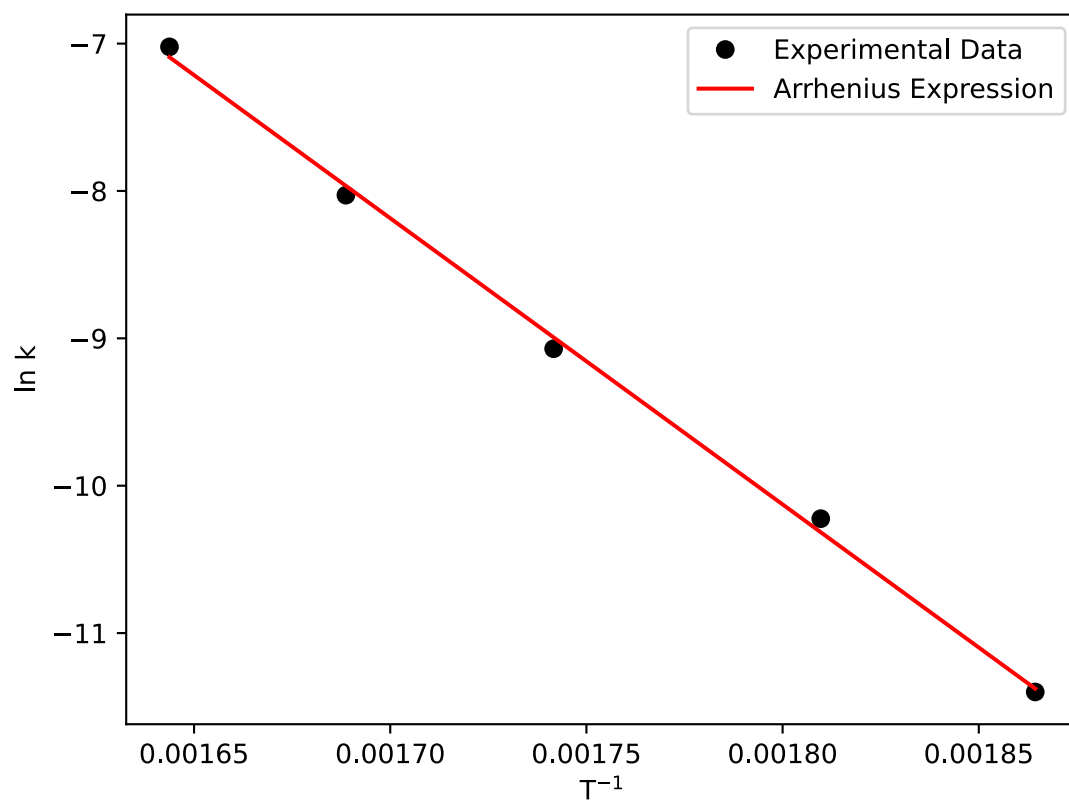


Figure 1. Arrhenius plot based on the experimental data presented in Table 1.